5-Hepten-2-amine, N,6-dimethyl-

Other names:	4-Hexenylamine, N,1,5-trimethyl-
	Isometheptene
	Isonyl
	6-Methylamino-2-methyl-2-heptene
	2-Methyl-6-methylamino-2-heptene
	Octanil
	Octin
	Octinum
	Octon
	N,1,5-Trimethyl-4-hexenylamine
	6-Methylamino-2-methylheptene
	Octine
Inchi:	InChI=1S/C9H19N/c1-8(2)6-5-7-9(3)10-4/h6,9-10H,5,7H2,1-4H3
InchiKey:	XVQUOJBERHHONY-UHFFFAOYSA-N
Formula:	C9H19N
SMILES:	CNC(C)CCC=C(C)C
Mol. weight [g/mol]:	141.25
CAS:	503-01-5

Physical Properties

Property code	Value	Unit	Source
gf	183.52	kJ/mol	Joback Method
hf	-73.47	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	41.71	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.341		Crippen Method
mcvol	143.350	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1055.70		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1016.00		NIST Webbook

rinpol	1016.00		NIST Webbook
rinpol	1054.10		NIST Webbook
rinpol	1029.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1289.00		NIST Webbook
ripol	1280.00		NIST Webbook
tb	459.09	K	Joback Method
tc	641.36	K	Joback Method
tf	209.81	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.84	J/mol×K	459.09	Joback Method
cpg	321.82	J/mol×K	489.47	Joback Method
cpg	336.10	J/mol×K	519.85	Joback Method
cpg	349.71	J/mol×K	550.22	Joback Method
cpg	362.68	J/mol×K	580.60	Joback Method
cpg	375.04	J/mol×K	610.98	Joback Method
cpg	386.80	J/mol×K	641.36	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C503015&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume